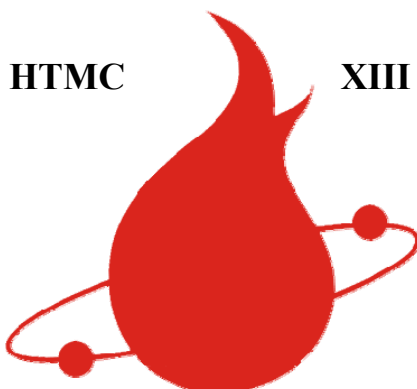




HTMC-13
High Temperature Materials Chemistry
September 14-18, 2009
University of California, Davis, CA, 95616, USA



Tuesday, September 15, 8:00 am, Giedt Hall – Conference Registration

AGENDA

Tuesday, September 15, 2009

8:00-8:45 am *Registration, Breakfast and Coffee, Giedt Hall*

Conference location: Giedt Hall

Room 1001

8:45-9:00 am Welcome and Announcements, **Alexandra Navrotsky**, University of California, Davis, USA

9:00-9:10 am Welcome Remarks, **Winston Ko**, Dean of Mathematical and Physical Sciences, University of California, Davis, USA

9:10-9:20 am Welcome and a Historical Perspective of HTMC, **Adolf Mikula**, University of Vienna, Austria

9:20-9:30 am Welcome and IUPAC Perspective, **Gerd Rosenblatt**, Lawrence Berkeley National Laboratory, USA

9:30-10:30 am Invited Lecture: **Jonathan Stebbins**, Stanford University, USA
PRESSURE AND TEMPERATURE EFFECTS ON THE STRUCTURE OF OXIDE MELTS

10:30-11:00 am *Coffee Break*

Parallel Sessions**Room 1001****Metals and Alloys**

(Session Chair: Kristina Lilova, USA)

Room 1002**Materials for Energy Applications**

(Session Chair: Nissim Navi, Israel)

11:00-11:20 am

Sergio Brutti, ItalyTHERMODYNAMICS AT FINITE TEMPERATURES OF THE INTERMEDIATE PHASES IN THE Re-B SYSTEM BY DENSITY FUNCTIONAL THEORY AND PERTURBATIONAL DFT CALCULATIONS
Sergio Brutti, Guido Gigli, Andrea Ciccio**Theodore Besmann**, USAAPPLICATION OF THERMOCHEMICAL MODELING OF TRANSURANIC OXIDE NUCLEAR FUELS
Theodore M. Besmann

11:20-11:40 am

Andrea Ciccio, ItalyAN EXPERIMENTAL AND COMPUTATIONAL STUDY OF BISMUTH-CONTAINING INTERMETALLIC MOLECULES
Andrea Ciccio, Marco Lauricella, and Guido Gigli**Christine Guéneau**, FranceCOMPATIBILITY AT HIGH TEMPERATURE BETWEEN CANDIDATE FUEL MATERIALS FOR GAS COOLED FAST REACTORS
Christine Guéneau, Alexandre Berche, S. Chatain, S. Gossé, Cyril Rado, Jacques Lechelle, Jean-Christophe Dumas, Chantal Martial, Nathalie Dupin, Bo Sundman

11:40 am-12:00 pm

Stephane Gossé, FranceTHERMODYNAMIC STUDY OF THE PALLADIUM-RUTHENIUM-TELLURIUM SYSTEM
S. Gossé, C. Guéneau, S. Chatain**Franck De Bruycker**, GermanyHIGH TEMPERATURE STUDIES ON CARBIDE SYSTEMS FOR GENERATION IV NUCLEAR FUEL
F. De Bruycker, K. Boboridis, R. Eloirdi, D. Manara, O. Tougait, H. Noël

12:00-12:20 pm

Herbert Ipser, AustriaNi-P-Sn TERNARY SYSTEM AND BINARY SUBSYSTEMS: PHASE EQUILIBRIA AND THERMOCHEMISTRY
Herbert Ipser, Clemens Schmetterer, and Rajesh Ganesan**Tanghong Yi**, USANEW ZINTL PHASE CaFe_4As_3 FOR THERMOELECTRIC APPLICATION
Tanghong Yi, Adam Dioguardi, Nicholas Curro, Susan Kauzlarich

12:20-1:40 pm

*Lunch at Giedt Hall***Room 1001**

1:40-2:35 pm

Invited Lecture: **Tomas Diaz de la Rubia**, Lawrence Livermore National Laboratory, USA
ENERGY SECURITY, CLIMATE CHANGE AND LASER INERTIAL FUSION ENERGY

2:35-3:30 pm

Invited Lecture: **Jack Shlachter**, Los Alamos National Laboratory, USA
Achieving Transformational Materials Performance in a New Era of Science and a specific facility vision: MaRIE - Matter Radiation Interactions in Extremes

3:30-4:00 pm

Coffee Break

Parallel Sessions**Room 1001**

(Session Chair: Gustavo Costa, USA)
Materials for Energy Applications

Room 1002

(Session Chair: Fen Xu, USA)
Carbides and Nitrides

4:00-4:20 pm

Nissim Navi, Israel

ENTHALPY OF MIXING OF $\text{Sr}_{(1-x)}\text{Ca}_x\text{TiO}_3$ AND
 $\text{Sr}_{(1-x)}\text{Ba}_x\text{TiO}_3$ PEROVSKITE SOLID
SOLUTIONS

N.Navi, J. Zabicky, G. Kimmel, E. Goncharov,
R. Shneck, M.H. Mintz, A. Navrotsky

Frezghi Kibrom, South Africa

THERMAL ETCHING OF 6H-SiC AND CVD-
POLY-CRYSTALLINE SiC

F.G. Kibrom, N.G. van der Berg, J.B. Malherbe
and A. Botha

4:20-4:40 pm

Speranta Tanasescu, Romania

THE INFLUENCE OF DOPANTS, OXYGEN
NONSTOICHIOMETRY AND PARTICLE SIZE
ON THE THERMODYNAMIC DATA OF
PEROVSKITE-TYPE MATERIALS

Speranta Tanasescu, Cornelia Marinescu, Anca
Sofronia, Florina Teodorescu, Alina Petcu

Hans Seifert, Germany

THERMODYNAMIC EVALUATION OF
LIQUID PHASE SINTERING OF SILICON
CARBIDE BY CALCULATION AND
EXPERIMENTS

Olga Fabrichnaya, Hans J. Seifert, Roland Neher,
Kristina Brandt, Mathias Herrmann

4:40-5:00 pm

Miloš Nevřiva, Czech Republic

THERMOCHEMICAL STUDIES OF MIXED
OXIDES IN THE Bi-Sr-Nb-O SYSTEM

Miloš Nevřiva and Jindřich Leitner

Andre Levchenko, USA

OXIDATION CALORIMETRY AND
THERMAL ANALYSIS OF MATERIALS: A
CARBON NANOTUBES STUDY

Andre A. Levchenko

5:00-5:20 pm

Wei Zhou, USA

THERMOCHEMISTRY OF HAFNIUM OXIDE
PHASES

W. Zhou, S.V. Ushakov, A. Navrotsky, T. Wang,
J. G. Ekerdt, A. A. Demkov

Emil Stoyanov, USA

NATURAL SILICON CARBIDE FROM
DIFFERENT GEOLOGICAL SETTINGS

Andrei A. Shiryaev, Emil Stoyanov, William L.
Griffin, and Hiroyuki Kagi

After 5:30 pm

*Dinner on your own***Wednesday, September 16, 2009**

8:00-8:30 am

Breakfast and Coffee, Giedt Hall

8:30-9:30 am

Room 1001Invited Lecture: **Yingwei Fei**, Carnegie Institution of Washington, USA

MELTING RELATIONS IN THE Fe-C-S-O SYSTEM AT HIGH PRESSURE: IMPLICATIONS FOR
PLANETARY CORES

9:30-10:30 am

Invited Lecture: **Kazunari Yamaura**, National Institute for Materials Science, Japan

POST-PEROVSKITE TRANSITION AND MAGNETIC AND CHARGE TRANSPORT PROPERTIES
OF THE CORRELATED $4d$ POST-PEROVSKITE CaRhO_3

10:30-11:00 am

Coffee Break

Parallel Sessions**Room 1001**

(Session Chair: Tatiana Shvareva, USA)
Materials for Energy Applications

Room 1002

(Session Chair: Hans Seifert, Germany)
Carbides and Nitrides

11:00-11:20 am

Chien-Ting Chen, USA
LOW TEMPERATURE PROTONIC
CONDUCTION IN NANOCRYSTALLINE
FLUORITE STRUCTURED SOLID
ELECTROLYTES
Hugo J. Avila-Paredes, Chien-Ting Chen,
Shizhong Wang, Manfred Martin, Zuhair A.
Munir, and Sangtae Kim

Nathan Jacobson, USA
THE ACTIVE OXIDATION OF SILICON
CARBIDE
Nathan S. Jacobson and Dwight L. Myers

11:20-11:40 am

Pragati Jain, USA
OXYGEN TRANSPORT IN SC-DOPED CERIA:
CATION (⁴⁵Sc) NMR SPECTROSCOPY AS A
PROBE OF ANIONIC CONDUCTIVITY
Hugo J. Avila-Paredes, Pragati Jain, Sabyasachi
Sen and Sangtae Kim

Dario Manara, Germany
HIGH-TEMPERATURE PHASE EQUILIBRIA
OF ZIRCONIUM CARBIDES: A LASER
HEATING STUDY
D. Manara, H. F. Jackson, C. Perinetti – Casoni,
W.E. Lee, L. Luzzi, P. M. Ossi, R.J.M. Konings

11:40 am-12:00 pm

Torsten Markus, Germany
MIXED IONIC ELECTRONIC CONDUCTING
(MIEC) PEROVSKITES FOR OXYFUEL
PROCESSES
Torsten, Markus, Anna Ellett, Annett Möbius,
Dominik Schlehuber, and Lorenz Singheiser

Emanuel Ionescu, Germany
SILICON OXYCARBIDE/HAFNIA CERAMIC
NANOCOMPOSITES – PREPARATION AND
HIGH-TEMPERATURE BEHAVIOR
Emanuel Ionescu, Benjamin Papendorf, Hans-
Joachim Kleebe, and Ralf Riedel

12:00-12:20 pm

Ravi Mohan Prasad, Germany
THERMORESISTANT AMORPHOUS
CERAMIC MEMBRANES FOR HYDROGEN
PURIFICATION
Ravi Mohan Prasad, Aleksander Gurlo,
Yuji Iwamoto and Ralf Riedel

Adolf Mikula, Austria
EXPERIMENTAL METHODS TO DETERMINE
THERMODYNAMIC PROPERTIES OF
TERNARY ALLOYS
Adolf Mikula

12:20-1:40 pm

Lunch at the Gunrock Pub

1:40-2:40 pm

Room 1001

Invited Lecture: **Suzana Fries**, Ruhr University Bochum, Germany
NI-BASE SUPERALLOYS: WHEN BASIC KNOWLEDGE MEETS APPLICATIONS

Parallel Sessions**Room 1001**

**Geological Applications and
High Pressure**
(Session Chair: Sarah Gaudio, USA)

Room 1002

Metals and Alloys
(Session Chair: Masao Morishita, Japan)

- 2:40-3:00 pm **Andrei Chychko**, Sweden
THE HEAT EFFECTS OF THE SLAG
FOAMING CAUSED BY CARBONATES
DECOMPOSITION
Andrei Chychko and Seshadri Seetharaman
- 2:40-3:00 pm **Stefan Hoffmann**, Germany
MS-TG-DTA UNDER INERT CONDITIONS
Stefan Hoffmann and Rüdiger Kniep
- 3:00-3:20 pm **Charles Lesher**, USA
VOLUMETRIC PROPERTIES OF
AMORPHOUS MATERIALS AT HIGH
PRESSURE BY X-RAY
MICROTOMOGRAPHY AND
ADSORPTION
C.E. Lesher, A. N. Clark, S.J. Gaudio, A. A.
Clark, Y. Wang
- 3:00-3:20 pm **Sergey Ushakov**, USA
CALORIMETRY AT ULTRA-HIGH
TEMPERATURES:
NEW RESULTS ON REFRACTORY OXIDES
AND INSTRUMENTATION DEVELOPMENT
Sergey V. Ushakov and Alexandra Navrotsky
- 3:20-3:40 pm **Anwar Hushur**, USA
HIGH-TEMPERATURE BRILLOUIN
SCATTERING STUDY OF HAPLOGRANITE
SYSTEM: MEASUREMENTS OF T_g
Anwar Hushur, Murli H. Manghnani, Donald B.
Dingwell, and Quentin Williams
- 3:20-3:40 pm **Masao Morishita**, Japan
SYMMETRY OF THERMODYNAMIC
STRUCTURE FROM ABSOLUTE ZERO TO
HIGH TEMPERATURE IN THE
MAGNESIUM-ZINC BINARY SYSTEM
Masao Morishita, Hiroaki Yamamoto, Sinichi
Shikada, Minoru Kusomoto, Yasutomoto
Matsumoto
- 4:00 pm *Buses leave for Old Sacramento excursion and Banquet Dinner at the Firehouse
(optional and must have ticket to attend)*
- 6:30 pm *Dinner at the Firehouse, located at 1112 Second Street, Old Sacramento, California*
- 10:00 pm *Buses return to Davis*

Thursday, September 17, 2009

- 8:00-8:30 am *Breakfast and Coffee, Giedt Hall*
- 8:30-9:30 am Perspective: **Alexandra Navrotsky**, University of California, Davis, USA
ENERGY, ENVIRONMENT, AND HIGH TEMPERATURE MATERIALS
- 9:30-10:30 am Invited Lecture: **Sharon Webb**, Georg-August University, Goettingen, Germany
CONFIGURATIONAL HEAT CAPACITY, VISCOSITY AND STRUCTURE OF SILICATE MELTS
- 10:30-11:00 am *Coffee Break*

Parallel Sessions	Room 1001 (Session Chair: Charles Lesher, USA) Geological Applications and High Pressure	Room 1002 (Session Chair: Emil Stoyanov, USA) Carbides, Nitrides, Sulfides
11:00-11:20 am	Lara O'Dwyer Brown, USA VISCOSITY OF NATURALLY OCCURRING SILICATE LIQUIDS AT HIGH PRESSURE Lara O'Dwyer Brown and Charles E. Lesher	Gabriela Mera, Germany POLYMER-DERIVED CARBON-RICH SiCN CERAMICS – SYNTHESIS, PROPERTIES AND APPLICATIONS Gabriela Mera and Ralf Riedel
11:20-11:40 am	Sarah Gaudio, USA STRUCTURAL RELAXATION PHENOMENA IN AMORPHOUS SILICATES AT HIGH PRESSURE AND TEMPERATURE Sarah J. Gaudio, Charles E. Lesher, and Sabyasachi Sen	Nisarg Bhatt, India DEBYE TEMPERATURE, MEAN-SQUARE DISPLACEMENT AND HIGH-PRESSURE MELTING CURVE FOR fcc-Pb N. K. Bhatt, P. R. Vyas and A. R. Jani
11:40 am-12:00 pm	Bin Xu, USA THEORETICAL STUDY ON THE THERMODYNAMIC PROPERTIES OF Al ₂ O ₃ and Si ₃ N ₄ AT HIGH PRESSURE Bin Xu and Jianjun Dong	Aitana Tamayo, Germany SAXS ANALYSIS OF NANOSTRUCTURED C-RICH SiCN CERAMICS Aitana Tamayo, Gabriela Mera, Hong Nguyen, Ralf Riedel and Sabyasachi Sen
12:00-12:20 pm	Masaki Akaogi HIGH-PRESSURE POST-PEROVSKITE TRANSITIONS OF CaMO ₃ Masaki Akaogi, Yuichi Shirako, Hiroshi Kojitani, Sayaka Takamori, Kazunari Yamaura, Eiji Takayama-Muromachi	Tarun Bera, USA Cs _{n-1} BiAs _n S _{2n+1} (n = 3 to 9) QUARternary CHALCOGENIDE GLASSES Tarun K. Bera and Mercouri G. Kanatzidis
12:20-1:40 pm	<i>Lunch at Giedt Hall</i>	
1:40-2:40 pm	Room 1001 Invited Lecture: Ricardo Castro , University of California, Davis, USA CALORIMETRIC MEASUREMENT OF THE INTERFACE ENERGY USING NANOPARTICLES	
3:00-5:30 pm	Room 1007 Poster Sessions and Refreshments Dhanesh Chandra, USA HYDROGEN STORAGE IN Li AMIDE-IMIDE COMPLEX HYDRIDES Dhanesh Chandra, Wen-Ming Chien, Josh Lamb, Klaus Yvon, Nicola Penin, Radovan Cerny, Michel Latroche, Ashfia Huq, James Richardson, and Evan Maxey	

Dhanesh Chandra, USA

VAPOR PRESSURE MEASUREMENTS OF GAS GENERATOR MATERIALS: PURE AMMONIUM NITRATE AND THE AMMONIUM NITRATE-POTASSIUM NITRATE SOLID SOLUTION BY TORSION-EFFUSION METHOD

Wen-Ming Chien, Dhanesh Chandra, K.H. Lau and A.M. Helmy

Emanuel Ionescu, Germany

SILICON OXYCARBIDE/ZIRCONIA CERAMIC NANOCOMPOSITES WITH EXCELLENT HIGH-TEMPERATURE BEHAVIOR

Christoph Linck and Ralf Riedel

Nathan Jacobson, USA

THE GOLD-CARBON EUTECTIC

Nathan S. Jacobson and Evan H. Copland

Glen Kessinger, USA

THE HIGH TEMPERATURE REACTIVITY OF Li₂O

G. Kessinger, A. R. Jurgensen, D. M. Missimer, and J. S. Morrell

Frezghi Kibrom, South Africa

THERMAL ETCHING OF 6H-SiC AND CVD-POLY-CRYSTALLINE SiC

F. Kibrom, N.G. van der Berg, J.B. Malherbe and A. Botha

Torsten Markus, Germany

THERMODYNAMIC PROPERTIES OF Al-Cr-Fe ALLOYS EXPERIMENTAL INVESTIGATION BY KNUDSEN EFFUSION MASS SPECTROMETRY

Torsten, Markus, Vladimir Motalov, Dieter Kath, and Lorenz Singheiser

Masao Morishita, Japan

TUNGSTEN CARBIDE INVOLVING METAL DOMAINS COMPOSED OF IRON AND MANGANESE

Masao Morishita, Hiroaki Yamamoto, Ai Onoue, Masaaki Ikebe, Masahiro Iwasaki, Hidefumi Yanagida and Hiroshi Nishimaki

Tae-Jin Park, USA

THERMOCHEMISTRY OF TITANOSILICATE MATERIALS RELEVANT TO NUCLEAR ENERGY WASTE FORMS

Tae-Jin Park, Tina M. Nenoff, Terry J. Garino, James L. Krumhansl, Mark J. Davis, Paula Vullo and Alexandra Navrotsky

Vilma Petkova, Bulgaria

COMPARATIVE STUDY OF THE THERMAL BEHAVIOR OF MECHANOACTIVATED NATURAL APATITES FROM TUNIS, BULGARIA, ESTONIA, AND UZBEKISTAN

V. Petkova, Yu. Kalvachev, T. Kaljuvee, O. Petrov, K. Tonsuaadu, V. Yaneva, I. Dombalov, Y. Pelovski

Vilma Petkova, Bulgaria

INFLUENCE OF GASEOUS MEDIUM ON THE PROCESS OF THERMAL DECOMPOSITION OF IRON SULFATES

V. Petkova, Y. Pelovski, Yu. Kalvachev, D. Paneva, I. Mitov

Speranta Tanasescu, Romania

HIGH TEMPERATURE THERMODYNAMIC PROPERTIES OF SOME MULTIFERROIC CERAMICS
BASED ON BIFEO₃

S. Tanasescu, C. Marinescu, A. Sofronia, A. Ianculescu, L. Mitoseriu

After 5:30 pm

Dinner on your own

Friday, September 18, 2009

8:00-9:00 am

Breakfast and Coffee, Giedt Hall

Room 1001

(Session Chairs: Wei Zhou, USA and Sergey Ushakov, USA)

Energy and Miscellaneous

9:00-9:20 am

Amir Tavakoli, Germany

KINETIC EFFECT OF BORON ON THE DEGRADATION OF Si₃N₄ IN
Si-(B-)C-N POLYMER-DERIVED CERAMICS

Amir H. Tavakoli, Peter Gerstel, Jerzy A. Golczewski, Joachim Bill

9:20-9:40 am

Gustavo Costa, USA

SURFACE ENERGETICS OF CUBIC YTTRIA STABILIZED ZIRCONIA NANOPOWDERS

G. C. C. Costa, S. V. Ushakov, A. Navrotsky and R. Muccillo

9:40-10:00 am

Zdeněk Sofer, Czech Republic

PREPARATION OF ZnO CRYSTALS DOPED BY TRANSITION METALS

Zdeněk Sofer, David Sedmidubský, Jindřich Leitner, Štěpán Huber, Jiří Hejtmánek, Miroslav Maryško,
Karel Jurek

10:00-10:20 am

Kristina Lilova, USA

CALORIMETRIC STUDIES OF Fe(II)-BEARING COMPOUNDS AND APPLICATION TO THE
THERMODYNAMICS OF THE Fe-Ti-O SYSTEM

Kristina I. Lilova, Alexandra Navrotsky

10:20-10:40 am

Coffee Break

10:40-11:00 am

John Roudebush, USA

THE EFFECT OF GRAIN SIZE ON THE HIGH TEMPERATURE THERMOELECTRIC
PROPERTIES OF THE TYPE-I Clathrate, Ba₈Al₁₀Si₃₆

John H. Roudebush, Herbert Sassik, Andrey Prokofiev, Silke Paschen and Susan Kauzlarich

11:00-11:20 am

Xianran Xing, China

THERMAL EXPANSION AND THERMAL CONTRACTION IN LEAD-BASED PEROVSKITES

Xianran Xing, Jun Chen, Penghao Hu, Jinxia Deng

11:20-11:40 am

Jun Chen, China

STRUCTURE OF HIGH-TC PIEZOELECTRIC PbTiO₃-BiMeO₃

Jun Chen, Penghao Hu, Jinxia Deng, and Xianran Xing

11:40 am-12:00 pm Closing Remarks – **Alexandra Navrotsky**, University of California, Davis, USA

12:00-1:30 pm *Lunch at Giedt Hall*

1:30 pm Optional Tour of Peter A. Rock Thermochemistry Laboratory and other UC Davis Labs